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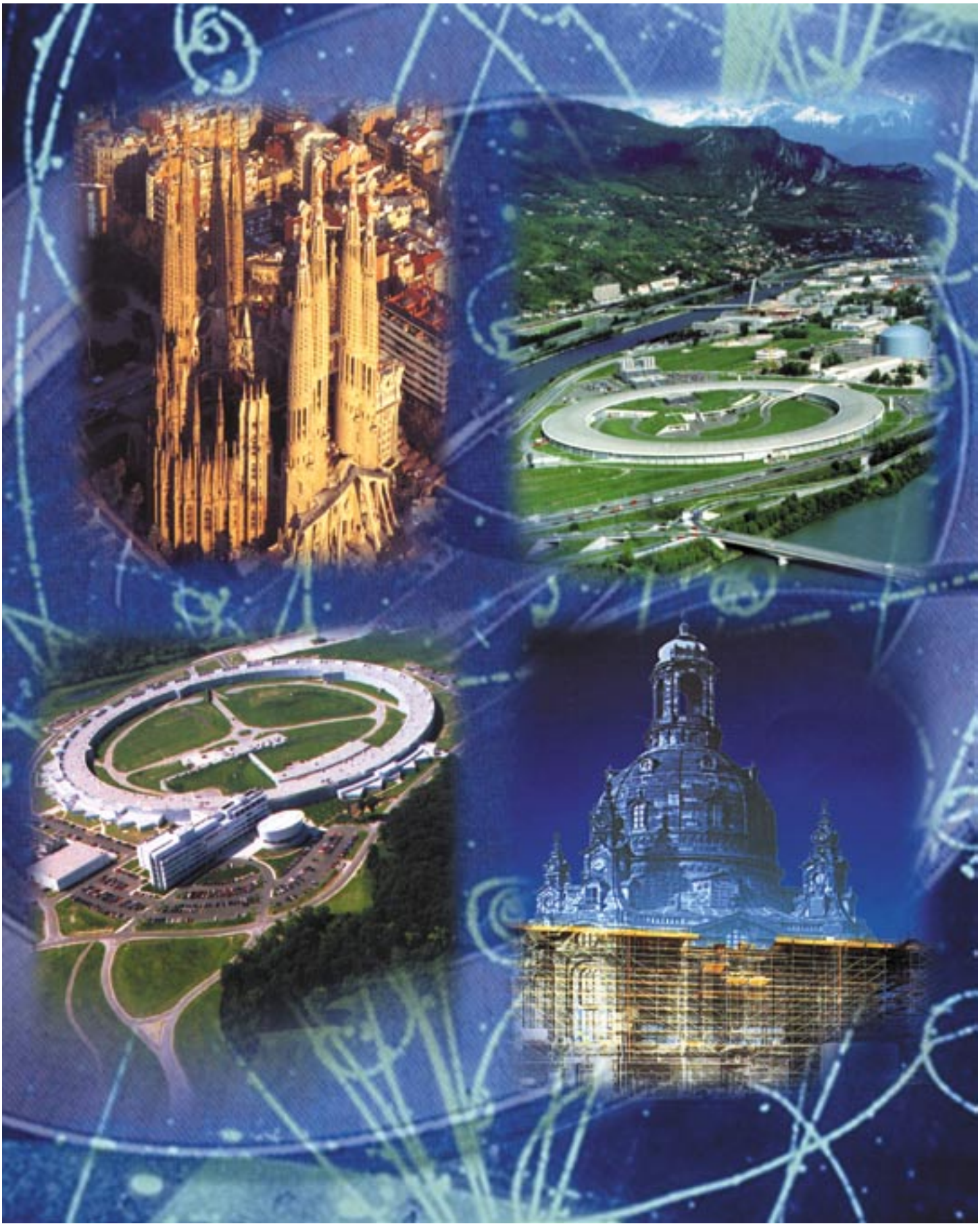

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Articles by e-mail or on diskettes are especially welcome. Deadlines for newsletter contributions are: February 1 (Spring issue), May 1 (Summer), August 1 (Fall), and November 1 (Winter). Matters pertaining to advertisements, membership inquiries, or use of the ACA mailing list should be addressed to:

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President's Column

Last year was my first on ACA Council and it was a very positive experience. We clearly benefited from the wisdom and good spirit with which Connie Chidester led our organization. As Past President, Connie will remain on Council through 2001. We will miss Abe Clearfield as he rotates off Council and we welcome new members: VP: Charlie Carter and Treasurer-Elect: Doug Ohlendorf.

Thinking about Neutrons -

The brilliance and tunability of the x-rays which experimentalists access at synchrotron sources around the world are now appreciated by most ACA members and for many, synchrotron radiation forms an integral component of their research. At the University of Saskatchewan in Saskatoon, the Canadian Light Source is expected to deliver its first photons early in 2004 (http://www.cls.usask.ca). Neutrons have likewise always been highly valued by the crystallographic and scattering communities, but the relatively weak flux of neutron beams and requirement for significantly larger crystals have, for some, been limiting factors for their use in structural science. Nevertheless, things are changing in the new millennium. The protein crystallography station at the Los Alamos National Labs Neutron Science Center (http://www.lansce.lanl.gov) has just come on line and Oak Ridge National Labs in Tennessee, in partnership with 5 other DOE laboratories, will be the site of a new 2MW Spallation Neutron Source (SNS), making it a premier global center and user facility for international, multidisciplinary collaborations in neutron science. A proposal for a 5 MW European Spallation Source, the ESS (http://www.ess-europe.de) is under active consideration and would complement existing facilities such as ISIS in England (http://www.isis.rl.ac.uk) and the IIL in France (http://www.ill.fr). In Japan, the Hadron Facility is expected to be operational next year and

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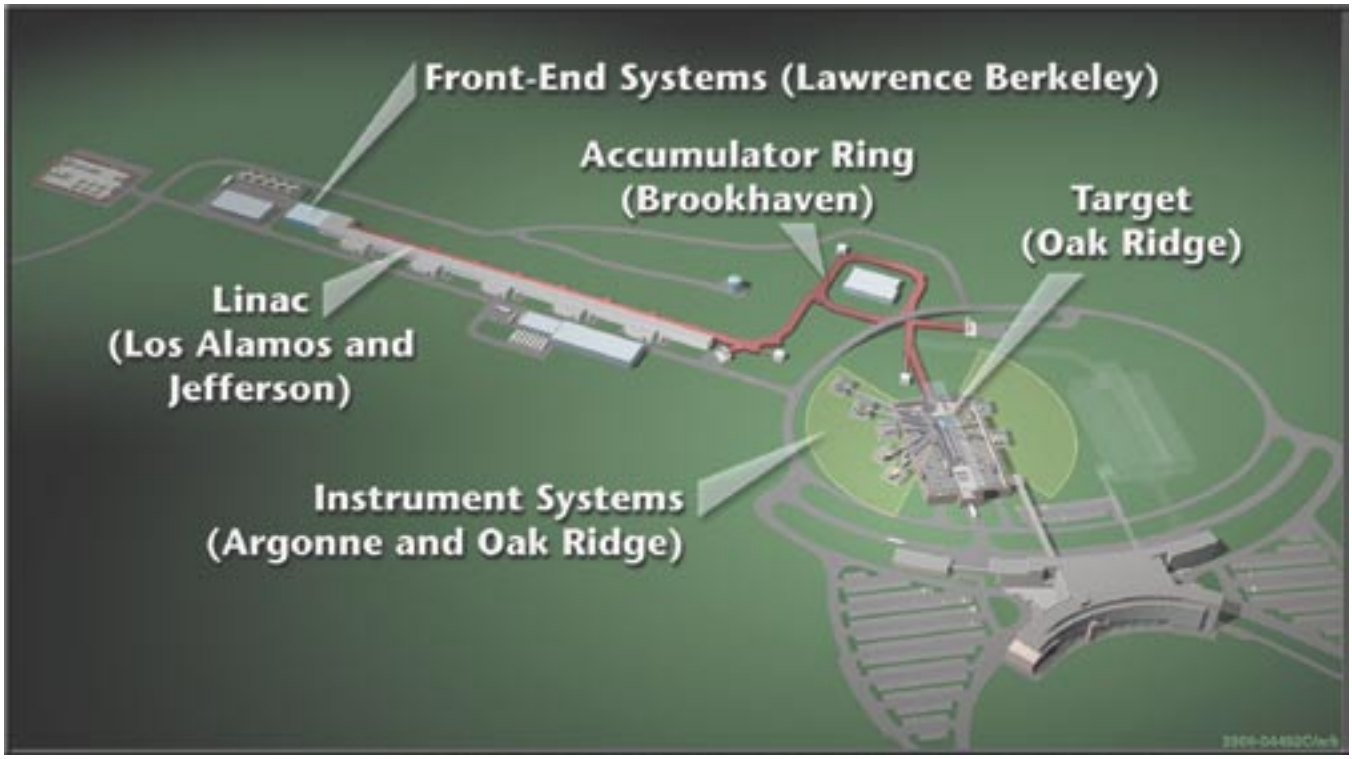
in 2007, look for neutrons from an 8 MW source to be developed by the Japanese Atomic Energy Research Institute.

In 2006, the SNS at Oak Ridge (http://www.sns.gov) will be the center of major research activities which will include small angle scattering, powder diffraction, reflectometry, low resolution diffraction, membrane scattering and small molecule structure determination. Construction is now underway. In December 2000, I attended a meeting in Knoxville on the additional possibility of using the SNS for macromolecular crystallography. A report with the important issues, outcomes and action items from this workshop can be found in the Newsletter. What excited me about the Knoxville meeting were the very real possibilities of locating hydrogen and deuterium atoms in protein or nucleic acid structures from crystals of no more than half a millimeter in each dimension with advances in image plates and area detector technologies which will also lead to significantly reduced data collection times. Hence the SNS will also have potential for impact on additional areas such as those which target important advances in understanding enzyme mechanisms, macromolecular solvation, ligand binding and structure-based drug design. Overall I am confident that the future of the SNS will capture the imagination of all ACA members and for many, renew their interest in neutron scattering and diffraction. A follow-up workshop around this theme will be held at this year's ACA meeting in LA. Those interested can contact Gerry Bunick (bunickgj@ornl.gov) and Leif Hanson (hansoll@bio.lsd.ornl.gov), or perhaps follow details from the ACA homepage. In addition, the Neutron Scattering SIG has organized an impressive series of sessions for the LA meeting which feature an international panel of speakers. I urge ACA members and their colleagues who wish to benefit from the neutrons generated at the SNS and the other new facilities to work together and be prepared to demonstrate support for their promising impact on structural science. The timing and technologies are now clearly ripe for new opportunities using neutrons.

Looking forward to our meeting in LA !

Bill Stallings



Schematic Drawing of the Spallation Neutron Source (SNS)

Workshop on Macromolecular Single Crystal Diffraction at The Spallation Neutron Source

Neutron diffraction provides important and unique information for macromolecular structure–function studies. Hydrogens comprise roughly half the atoms of biological materials such as proteins and DNA, and hydrogen ions supply the primary motive force in the molecular actions of such fundamental biological processes as metabolism and reproduction. The ability of neutrons to reveal the positions of hydrogens even at moderate resolution (2.5 Å) is the foundation of the scientific justification for neutron diffraction of biological samples. Although other techniques may provide complementary information, none do it at such moderate resolution levels nor as conclusively as neutrons.

On December 18-19, 2000, a workshop was held in Knoxville, Tennessee to discuss single crystal neutron diffraction studies and the potential role of the Spallation Neutron Source (SNS) in the future of such studies. Presenters and participants included structural biologists, instrumentation specialists, administrators and microgravity-crystal growth experts from local, national, and international locales. Among the international participants were John Helliwell and Chick Wilson from Great Britain, Peter Timmins and Dean Myles from Grenoble, Nobuo Niimura and Ichiro Tanaka from Japan. Other presenters included Paul Langan from Los Alamos; Art Schultz from Argonne; Dan Carter from New Century Pharmaceuticals and Eddie Snell from MSFC in Huntsville; Chris Dealwis, of the University of Tennessee; and Thom Mason, Don Hutchinson, and Gerry Bunick from Oak Ridge. The workshop was co-sponsored by SNS and NASA. The local organizing committee included Gerry Bunick, Chris Dealwis, Leif Hanson and Jinkui Zhao.

Presentations were heard on the first day, including scientific advances with macromolecular neutron diffraction, the developments of neutron sources, detectors and beam lines world wide, and the role microgravity is playing in the growth of crystals suitable for neutron diffraction experiments. The potential role of macromolecular neutron diffraction at SNS has not been recognized, as illustrated even in local news media reports. Therefore, an important mission of the workshop was to inform both crystallographers and other biologists interested in structure-function studies of biomolecules on the merits of neutron diffraction studies, as a preamble to more widespread dissemination of information. There is coming a unique confluence of events that will provide both opportunities to grow large crystals (on the International Space Station) and to collect data at high flux neutron sources (ILL, ISIS, SNS and the proposed ESS).

The SNS will have a 2 megawatt power output: this about half the integrated power of ILL, but 50 times higher in peak power, and 12 times greater than that of the world's highest power spallation source, ISIS, at the Rutherford Appleton Laboratory in Great Britain. The SNS is designed so that future power upgrades can be made with relatively modest expenditures. Site excavation has been completed and the first neutrons are expected in June of 2006. Currently one target station is funded, the high power target station (HPTS), and funding is being sought for the construction of a second target station, the long wavelength target station (LWTS). Further information on the source is available at the SNS website (www.sns.gov). Although a small molecule instrument equipped with furnaces and refrigerators, as well as magnets and high-pressure devices is planned, at present, no instrumentation for macromolecular crystallography is in development. Instrumentation for one potential macromolecular crystallography beam line has been proposed in the yet to be approved second target station. Details on this device are included in proposal to the National Science Foundation for funding the LWTS (www.sns.anl.gov/LWTS/NSF_LWTS_Proposal.pdf).

The scientific case for neutron diffraction was presented by the keynote speaker, John Helliwell, whose research into the basis of sugar recognition by concanavalin A (con A) has encompassed extensive synchrotron X-ray and neutron data collection. John envisions the SNS becoming the state of the art for neutron users and the test bed for future spallation sources and instrumentation. Europeans view the SNS as a justification for construction of the European Spallation Source (ESS). As Europe watches developments with SNS, continued upgrades of existing neutron facilities are underway both in Great Britain and on the continent. These upgrades include a new area detector for the D19 beam line at ILL and upgrades of neutron Laue time-of-flight instruments at ISIS, indicating a movement toward more protein crystallography for detailed analysis of hydrogen bonding and catalytic site structure.

The traditional basis for neutron diffraction is the ease with which accurate positions of hydrogens/deuterons can be determined in crystals of macromolecules. Both deuterium and oxygen scatter similarly in neutron diffraction experiments; solvent position and proton exchange can be readily identified from neutron diffraction data. A more recent rationale for neutron diffraction can be seen in the comparative diffraction data for con A between an ultra-high resolution X-ray cryostructure and a medium resolution neutron room temperature structure. The neutron data were collected at ILL from a D_2O soaked crystal of 3 mm x 2 mm x 1 mm. Data were collected in 10 days and were 89% complete to 2.4 Å. The neutron structure provided six times the number of well-determined waters (position and orientation) compared with the ultra-high resolution X-ray data (0.9 Å). Neutron diffraction determines bound waters more efficiently, and it should provide the primary means of identification of the positions of somewhat mobile waters in a protein structure [Habash et al., 1999]. Additional medium resolution neutron data features not seen in all but the highest resolution X-ray data are the short vs. long bond lengths for acidic side chains, which are uninterpretable at resolutions less than 1.2 Å.

Neutron diffraction data should have a major role in assisting future computational biology research, by providing

Jinkui Zhao (SNS) discussing options for diffraction instruments at SNS. (Left to right: Nobuo Niimura, Ichiro Tanaka, Tom Koetzle, Charles (Chick) Wilson, John Helliwell, Peter Timmins, Angus Wilkinson, and Lisa Edberg.

a structural data base for understanding the role of solvent in ligand interaction, and providing further needed information to understand the thermodynamics of ligand recognition from structural data. Such studies will have a direct impact on rational drug design, providing more accurate and complete molecular structures. Thermal parameter values for H and D atoms may also be assigned based on neutron diffraction data, for proteins that diffract to high resolution. To fully understand the water structure and proton exchange rates of native molecules, low temperature X-ray data must be compared with room temperature neutron data. Even at ultra-high resolution, X-rays are not good at distinguishing water molecules from monovalent cations (sodium, ammonium, potassium). It will not be possible to understand processes like RNA folding and catalysis, or DNA bending unless the positions and types of cations are identifiable.

Peter Timmins reported that unique information on the location of H atoms and water has been obtained by neutron fiber diffraction of biological polymers, including cellulose, hyaluronic acid, filamentous viruses, and DNA. For example, individual water positions along the DNA strand have been refined even at the low resolution of 3 Å. Other significant diffraction information can be obtained at low resolution including the localization of surfactants added to proteins. The detergent structure in integral membrane proteins has not been possible to determine in X-ray diffraction studies owing to the disorder of the surfactants in the unit cell. It has now been possible to resolve the detergent structure in crystals of OmpF porin of *E. coli* using neutron contrast matching studies [Pebay-Peyroula *et al.*, 1995]. Given that 40% of the genome is membrane-bound proteins, which are extremely difficult to crystallize, the strategic importance of such neutron studies in revealing the interactions of proteins and detergents cannot be emphasized enough.

Improvements in neutron sources, detector design and interpretation of multi-wavelength diffraction have improved the speed with which data can be collected. Detector improvements include the neutron image plate, which is currently in use in both Japan and Europe, a neutron area detector with 1mm pixel size being developed at Oak Ridge, and detector research at Brookhaven National Laboratory for the SNS project. Nobuo Niimura presented rubredoxin data (unit cell axes 34 Å x 35 Å x 44 Å; crystal size 2.6 mm x 1.7 mm x 1.0 mm) collected with a neutron image plate in 11 hrs. The resolution of the data is 1.5 Å and the refinement of the hydrogen positions at 1.5 Å is currently underway. At the Japanese Atomic Energy Research Institute (JAERI), the rule of thumb for data collection from macromolecular crystals is that each axis must be less than 100 Å. However, longer unit cell lengths can be accommodated if the other axes are smaller (i.e., 50 Å x 50 Å x 200 Å). The volume of the crystal must be = 2 mm^3, so 1.5 mm x 1.5 mm x 1.0 mm is around the current minimum acceptable crystal volume. Construction has started on the new BIX-4, the performance of which will be at least 3 times better than the present BIX-3. The necessary crystal volume should be ~1/3 that of BIX-3.

In addition to steady state neutron sources, several spallation sources are planning to contribute to biological neutron diffraction research. ISIS, at the Rutherford Appleton Laboratory, does not have a protein crystallography instrument in place, but the facility is currently undergoing upgrades consisting of a second target station, which will include such an instrument. In this country, the Protein Crystallography Station (PCS) at the Lujan Center source at the Los Alamos Neutron Sciences Center (LANSCE) produced its first neutron beam on a sample in the week prior to the conference. The PCS is a new diffraction instrument for protein crystallography, fiber, and membrane diffraction. This instrument, with a partially coupled water moderator, uses a large cylindrical position sensitive detector for collecting data. The detector has an active area of 3000 cm^2 and a resolution of 1.3 mm with

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a counting rate over 1 million counts/sec. A call for proposals at the LANSCE PCS will be issued in 2001.

As a result of microgravity studies supported by both NASA and the ESA, production of crystals sufficiently large for neutron diffraction studies could become commonplace. Dan Carter reported reliable growth of crystals with the 1 mm^3 volume needed for current neutron diffraction experiments for even such problematic proteins as bacteriorhodopsin. With the commissioning of the International Space Station, a permanent venue now exists that should be available to crystallographers interested in using microgravity for crystal growth. It is estimated that with the extended duration missions on the ISS, ~90% of proteins crystallized on orbit will reach the 1 mm^3 size range needed for neutron diffraction experiments. For example, on flight STS-89, a crystal of ferritin was grown with a volume of 10 mm^3. Neutron diffraction data to 2.7 Å has been collected at ILL from this crystal, 1 Å higher resolution than the diffraction limit of ground grown crystals. In studies reported by Eddie Snell, microgravity grown crystals are consistently larger and more physically perfect than those grown terrestrially. This physical perfection takes place on both short and long-range scales, and has been quantified using X-ray diffraction rocking-curve studies. In contrast, despite early optimistic claims cited in the BERAC report, the evidence suggests that crystals of sufficient quality to diffract to > 0.9 Å for determination of hydrogen positions occur only in ~1% of proteins sampled.

One significant application for proteins structures determined by neutron diffraction will come in the area of rational drug design. Chris Dealwis pointed out the practicality of this approach, discussing the problems associated with finding an agonist of angiotensin to bind with rennin, and how this study carried over to drug discovery of anti-HIV proteases. Both rennin and HIV protease belong to the general class of aspartic proteases, so named for the aspartic acid moieties which are an integral part of the catalytic site. A solvent molecule bound tightly to both aspartate carboxyl groups is presumed to take part in the catalytic mechanism. Currently proposed mechanisms are largely based on X-ray inhibitor structures, but the assignment of protonation states to the catalytic groups during the reaction differ. Since the active-site H atoms cannot be located by current X-ray analyses, their putative positions have so far been inferred from the local geometry of surrounding polar atoms. Thus, locating the crucial protons at the active site will provide important information to firmly establish the catalytic mechanism.

Members of the workshop taking part in the discussions held the second day of the meeting, from left to right are Craig Kundrot (NASA), Nobuo Niimura, Ichiro Tanaka, Tom Koetzle, Chick Wilson, John Helliwell, and Peter Timmins.

Enzyme structure and mechanism continue to be fertile ground for neutron crystallography, from the seminal study of the catalytic triad of trypsin [Kosiakoff & Spencer, 1981], to new studies of aspartic proteases. A recent report of the neutron diffraction structure of the fungal aspartic protease endothiapepsin by Cooper and Myles (2000) is a research milestone for several reasons. It represents the largest protein solved by neutron diffraction methods (33 kDa), and by establishing the positions of the catalytic protons, represents a route to the development of more effective inhibitors to aspartic proteases. The endothiapepsin structure is the beginning of what may be one of the more significant roles played by neutron diffraction studies.

The second day of the workshop was dedicated toward discussions of macromolecular crystallography at SNS. Three primary conclusions were reached because of these discussions:

1). The landscape of macromolecular neutron diffraction

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Jinkui Zhao, Art Schultz, Chris Dealwis and Gerry Bunick discussing instrument parameters and the need for two diffraction instruments by the macromolecular crystallographic community.

has undergone a significant positive alteration in the past three years. Although neutron data collection will never be described as high-throughput, based on flux projections and detector development, it should be possible at SNS to collect a complete neutron diffraction data set from a crystal of 1.0 mm^3 with a longest unit cell dimension of 100 Å within 1 week. This is comparable to the size of crystal and time period needed to complete data collection with most in-house X-ray systems. In the absence of dedicated equipment planned for macromolecular crystallography, it was the sense of the workshop participants that single crystal biological instrumentation must form an integral part of SNS future beamline planning.

2.) Future planning at SNS should at a minimum encompass two protein crystal diffraction instruments: at the High Power Target Station (HPTS) an instrument capable of collecting data from crystals with a maximum unit cell length of 100 Å, and at the Long Wavelength Target Station (LWTS) a device capable of resolving atomic positions from crystals with unit cell axes of 250 Å or less. This instrument should have additional capabilities for membrane, fiber, and low-resolution diffraction studies.

3.) Current proposals submitted to NSF for funding a LWTS at SNS include the second macromolecular device described earlier. Based on current instrumentation funding at HPTS, it appears that an independent development team might be needed to ensure the inclusion at SNS of the first instrument described earlier. The formation of a committee to submit a letter of intent (LOI) for a HPTS beamline and the identification of target agencies for funding the IDT is planned.

In addition to these other findings, it was felt that educational and outreach activities should to be undertaken to acquaint a new generation of crystallographers of the scientific merits of neutron diffraction and of the advances that have been made in recent years. To this end, the workshop participants will seek to make presentations at various national societies, including the American Crystallographic Association. Plans for the ACA 2001 annual meeting include a workshop on macromolecular neutron crystallography.

Leif Hanson and Gerry Bunick

Polycrystal Book Service Moves

We are pleased to announce that Polycrystal Book Service has been sold to Dr. Dan Carter, President, of New Century Pharmaceuticals, at 895 Martin Rd., S.W., Huntsville, Alabama 35824, USA. Dan and his great staff will be keeping Polycrystal going in its best traditions of service and flexibility to serve all crystallographers world-wide. Their new website is: Polycbs.com and the email address is polycbs@polycbs.com. Jean Reynolds is the primary contact and we know that you will enjoy working with her!

They also have a toll-free number — 888-628-5611

We are forwarding all unfilled catalog orders and all other miscellaneous information requests (from our old e-mail file) to them so that they can ensure you are on their list for future notices. The catalog is now on the website (something we couldn't do!) and you will find that the business has been updated for improved operations in this electronic environment.

Thank you for your business, your support and your friendship over the past fourteen years of our being the 4th generation of "Poly" — we'll miss you!

Wade and Mert Adams
Former Owners of Polycrystal Book Service
New personal email: wademert@cs.com

Call for Proposals for Future ACA Meeting Sites

ACA Council would be pleased to review preliminary proposals from ACA members for future ACA Meeting sites.

Proposals can be submitted to any member of Council or directly to Marcia Evans in the ACA Office in Buffalo (marcia@hwi.buffalo.edu).

A typical proposal would consist of a brief statement on why the proposed site would be appropriate for an ACA meeting. For those interested in further details, a summary of the space and other requirements for a typical ACA meeting are available from the ACA Office in Buffalo.

2001 Ludo Frevel Crystallography Scholarship Recipients Announced

The ICDD Ludo Frevel Crystallography Scholarship Committee has selected six winners for the 2001 Scholarship program. They are: James Lettieri, of The Pennsylvania State University, in University Park, Pennsylvania, with research involving "Ferroelectric Anisotropy and Integration of SrBi Ta O ;" Meitian Wang, of the University of Alberta, in Edmonton, Alberta, Canada, with exploration into "Developing Structural Principles for New Ternary Metal-Rich Pnictides;" Christina DeWitt, of the Oklahoma Medical Research Foundation, in Oklahoma City, Oklahoma, with a major interest in "Determining the Structures of an Fc Derived from a Human Ig G1 (κ) Antibody;" Christine McCracken, of the University of Manitoba, in Winnipeg, Manitoba, Canada, with studies focusing on "The Crystallography and Chemistry of Tourmaline;" Maxim V. Lobanov, of the Moscow State University, in Moscow, Russia, with research concerning "Structural Studies of Low-Dimensional Magnetic Mn Oxides as Possible CMR Materials;" and Jennifer Stone, of the Oregon State University, in Corvallis, Oregon, who's investigating "Structural Studies of High-Power Optical Materials."

The ICDD will present each of these students with a check for $2,250 to help them continue their studies in their selected fields of crystallographic research.

Helen M. McDonnell

Correction: Additions to Donors List

Lee Daniels should have been listed as a donor to the Etter Award fund in the Fall Issue of the Newsletter. We apologize for the omission.

Awards to Prof. G.R. Desiraju

Professor Gautam R. Desiraju has recently received the following awards.

(1) Third World Academy of Sciences (TWAS) Award in Chemistry for 2000. This will be presented later this year and consists of a check for $10,000 and a citation which will read:

"For his pioneering contributions to the area of crystal engineering, the designed synthesis of solid state supramolecular entities, and for increasing the awareness in the properties and consequences of the weak hydrogen bond".

(2) Alexander von Humboldt Research Award. This is the highest award of the Humboldt Foundation, and is very well-known in the U.S., from where a number of researchers have been thus honored. Prof. Desiraju recently spent a month in Essen (with Roland Boese) under the scope of this prize.

IMCA-CAT Announces Independent Investigator Program

The Industrial Macromolecular Crystallography Association Collaborative Access Team (IMCA-CAT) announces the initiation of its Independent Investigator Program on its undulator insertion-device beamline, 17-ID, at the Advanced Photon Source, beginning October 1, 2000. The beamline is currently suitable for monochromatic data collections in a wavelength range of 0.82 to 2.4 Å, and semi-automated data collections at multiple wavelengths for MAD experiments. If you are an independent investigator seeking beam time for an individual macromolecular crystal structure project, or represent a collection of investigators undertaking a larger program of macromolecular structure determinations, such as multiple investigators from a single institution, or a structural genomics initiative, you may submit an application via the APS at http://www.aps.anl.gov/xfd/communicator/useroffice/II_proposal.html. For further information, please contact Dr. Andrew J. Howard, CAT Director, at howard@iit.edu or 630-252-0534.

Rheometric Scientific Acquires Protein Solutions

Rheometric Scientific, Inc. announced recently that it has acquired 100% of Protein Solutions, Inc.(PSI) and its UK affiliate, Protein Solutions, Ltd. PSI, based in Charlottesville, VA, is a leading manufacturer and marketer of Dynamic Laser Light Scattering (DLS) instrumentation, software and services. PSI is a recognized leader in the application of light scattering techniques for biomolecular characterization. PSI's products are based on a proprietary, patented technology to which PSI has an application exclusive license.

The PSI DLS technology employs sophisticated optical components and advanced digital signal processing to measure molecular physical properties such as size, mass, and diffusion. Pharmaceutical, biotechnology, and government funded research and development laboratories use this information to gain a better understanding of the stability and conformation of purified biomolecules. PSI products are optimized for specialized applications in protein science including biotherapeutic drug development, applied three-dimensional protein structure analysis, and developing structural genomics initiatives.

Rheometric Scientific, founded in 1970, manufactures instrumentation and provides laboratory services for material characterization. The Company's products and services are sold to numerous markets such as the petrochemical industry, academic and government research laboratories, and the food, pharmaceutical, biotechnology, and semiconductor industries worldwide. The Company is headquartered in Piscataway, new Jersey, and has operations in the United Kingdom, Germany, France, italy and Japan. More information about Rheometric Scientific can be found at www.rheosci.com. Information about PSI can be found at www.protein-solutions.com.

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Selection of Professor James McDonald Stewart for the Fankuchen Memorial Award

James McDonald Stewart will receive the 2001 Fankuchen Memorial Award, which recognizes an outstanding crystallographer who is known to be an effective teacher of crystallography. Jim had a long (1961-1998) and distinguished teaching and research career in the Department of Chemistry and Biochemistry at the University of Maryland. His career spanned the era in which the way that crystal structures are solved underwent a profound change, and Jim was one of the leaders in this revolution. As the major developer and coordinator of the XRAY and XTAL crystallographic software packages, Jim was an outstanding innovator in large-scale computing techniques. From the '60s through the '80s, his software efforts were the benchmarks for crystallographic computing and data standards, and they also influenced the design of software in other scientific disciplines such as the Gaussian software suite in computational chemistry. He was a leader in the implementation of computer applications to all aspects of crystallographic research—from powder to proteins—and his systematic approach to crystallographic computing was a major advance for the field of crystallography. He also popularized computational approaches through his important contributions to the ACA and IUCr teaching and computing schools, and all who were privileged to hear him on these occasions recognized his wonderful ability to teach crystallographic methods. In his teaching, Jim continually demonstrated the ability to motivate his students and the willingness to value their accomplishments ahead of his own. To Jim, teaching crystallography was as much about socializing as about pedagogy, and this is why he was so successful in meeting the challenges that new techniques and computer hardware posed. According to his students, he was the quintessential teacher: well-informed on his subject, intellectually curious about everything, clear in his explanations, patient towards students, and inspiring to young scientists. His zest for his subject was communicated in every interaction with his students, whether it was an explanation of space groups, the mechanics of a Fast Fourier Transform, or the arcana of data structures that would be transportable across computing platforms. He often spent a large number of non-classroom hours working with and for his students, who he treated like true colleagues by treating them with respect and consideration. His students often attribute a measure of their success to the preciseness of his instruction and the inspiration of his hard work. Outside the classroom, he was an innovator and inspirational teacher in computational crystallography. By creating the first comprehensive, transportable, and integrated system of crystallographic programs (The XRAY System), he revolutionized the field of crystallography. With a 'user friendly' system with one program flowing smoothly to the next, crystallographers could solve a broad spectrum of structures from start to finish. The availability of this computing package, coupled with the boundless energy and enthusiasm with which Jim would help anyone and everyone implement and understand the suite of programs, has been extremely important to the development of the field of crystallography. Many graduate students were educated in the field of crystallography as the XRAY System was both a teaching and a research tool, and the XRAY System error messages were a particularly useful guide to both crystallography and the correct use of the software. While the particular systems he developed are no longer widely used, the spirit that motivated them lives on in their successors. Jim Stewart's immense lifetime contributions to the development and teaching of computing methodologies have played a major part in the success and prominence that crystallography holds in science. His educational influence has reached far beyond the conventional classrooms. The committee considers that the Fankuchen Memorial Award would be an appropriate recognition for these most important contributions. (Members of the Fankuchen Award Selection Committee were: Jon Clardy, Kay Onan, Gerald Stubbs, and Jill Trewhella.)

Jon Clardy

Contributors to This Issue

Cele Abad-Zapatero, Mert Adams, Wade Adams, Gerry Bunick, Salvino Ciccariello, Jon Clardy, K.C. Cole, Patricia Coley, Tom Degnan, Gautam Desiraju, Marcia Evans, Judy Flippen-Anderson, Jerry Goodisman, Marv Hackert, Leif Hansen, Gernot Kostorz, Helen M. McDonnell, Gary Newton, John P. Rose, Bill Stallings, Ron Stenkamp, Bev Vincent, Alex Wlodawer.

Harry Brumberger (1926 - 2000)

Harry Brumberger, Professor of Chemistry at Syracuse University, and a pioneer in the field of small-angle scattering, died Friday November 10, 2000, in a Syracuse hospital, where he had been admitted for implantation of a pacemaker. He was 74 years old. He left behind his wife, Vilma, his children, Eva and Jesse, and one grandchild.

Harry had retired five years previously from the Chemistry Department, but had remained active in both teaching and research. Since his retirement, he had taught several courses in chemistry at Syracuse University and at the Environmental Science & Forestry College of SUNY, and was doing research on small-angle X-ray scattering from catalysts. He had recently been awarded a grant for this research by the Petroleum Research Foundation of the American Chemical Society.

Harry came to the United States from Vienna, Austria as a young teenager, with his parents, fleeing anti-Semitic persecution. Of his experiences in Austria he spoke little, except to those very close to him; painful as they must have been, he always held pre-1930s Austria in great affection. He attended high school, college and graduate school in New York City, and served in the U.S. army (ski troops). He earned bachelor's, master's and doctoral degrees at the Brooklyn Polytechnic Institute, as well as a master's degree from the Swiss Federal Institute of Technology (ETH) in Zurich. Harry's Ph. D. in Chemistry (1955) was directed by Rudolph Marcus, later a Nobel Prize winner in Chemistry, Harry being the first student to complete his doctorate under Marcus' direction. After his Ph.D., Harry left New York City for Cornell University in Ithaca, New York, where he worked as a post-doctoral associate with another Nobel Prize winner, Peter Debye. From Ithaca, it was a short jump to Syracuse, where he joined the Chemistry Department in 1957 as an assistant professor. He became associate professor in 1962 and professor in 1969. During his years at Syracuse University, he served as director of the Graduate Biophysics Program and of the Solid State Science and Technology Program. He was a visiting scholar at the University of Graz (Austria), the Weizmann Institute of Science (Israel), the University of Cambridge (England), and the Swiss Federal Institute of Technology (ETH) (Zurich, Switzerland).

Harry's research involved small-angle X-ray scattering from amorphous (non-crystalline) systems. Given the low-intensity sources available, the necessity for precise alignment and angular measurement, and the relatively featureless scattering curves obtained, this work required meticulous measurements, with great attention to detail and care in interpretation of experimental results. Harry became an expert in the field, respected internationally. He organized the first international conference on small-angle scattering, in Syracuse, and, in 1993, organized a NATO Advanced Institute on Small-Angle Scattering in Como, Italy. The Syracuse conference was the first in an ongoing series of triennial conferences, for which he continued to serve as a member of the advisory board. An often-invited speaker at international conferences, Harry edited a volume of papers on small-angle scattering and its applications, and published in the field at a constant rate throughout his years at Syracuse.

The research project in which he was engaged most recently involved small-angle scattering measurements on supported-metal catalysts, performed at the Cornell High-Energy Synchrotron. During the measurements, the metal-zeolite systems are exposed to oxidizing and reducing atmospheres in turn, as is done during the preparation of the catalysts, and particle sizes and surface areas are measured over time. The high intensity provided by the synchrotron X-ray source allows measurements over the entire angular range to be performed in seconds or minutes. Thus, one can learn when in the catalyst preparation process changes like sintering take place, and, eventually, how to vary conditions of preparation so as to obtain desired catalyst properties.

Harry Brumberger's publications are characterized by concision and clarity, reflecting both the carefully planned and executed experiments he reported, and the attention he gave in his writing to detail and to style. His elegant writing style came partly from his extensive reading in many areas, both scientific and extra-scientific. He always insisted on clarity and brevity, and spared no effort in making everything with his name on it as close to perfect as possible. This will long be remembered by collaborators on his papers, some of which never saw the light of publication because they fell short of his high standards.

The same desire for clarity influenced his teaching. He worked very hard to present the subject matter of his courses as clearly as possible, and was always ready to take whatever time was required to explain a difficult point to a student (or to a colleague). His adeptness at puncturing pomposity and signaling unclear thinking in others probably did not endear him to everyone. However, his teaching and advising were appreciated by the best students, and his advice was sought by colleagues all over the world, and not only on matters

continued on next page

related to his specialty. His counsel was also much appreciated on extra-scientific matters. Receiving correspondence from Harry was a great pleasure, due equally to the elegance of the writing style and the intelligence of the content.

It may be said that Harry Brumberger was a gentleman, a scientist, and a gentleman-scientist in the best sense of the word. While always thinking about his current scientific research, he refused to be limited to it. A truly educated and erudite man, he read widely in many areas, often impressing others by his knowledge. He had a particular interest in history, ancient and modern. In the months before his death, he was attending a course in Latin, with a view to studying some of the alchemical texts in the original. A few weeks before Harry's death, an article about the Cornell synchrotron and the research being done on it appeared in the local paper. The reporter, having met a scientist from Syracuse at the facility, interviewed Harry at some length. Harry told him about the joys of scientific research, and how they made all the hardships worthwhile (he and his helpers had to be present at their experiments night and day when "beam time" was available). His devotion to his research is one of the things we will long remember. We will also miss his elegance, wit, erudition, and the other qualities which made him such a great colleague and friend.

Jerry Goodisman, University of Syracuse, NY, U.S.A.;
Salvino Ciccariello, University of Padua, Italy;
Gernot Kostorz, ETH Zurich, Switzerland.

Arnold Beevers

Arnold Beevers died on January 16th, 2001, at the age of 92 in Scotland. A more complete description of his achievements will appear in future issues of this and/or the IUCr newsletter.

John L. Schlenker (1945-2000)

John, L. Schlenker, 55, of Anna, Illinois died suddenly at his home of a heart attack on September 20, 2000. John was a Senior Staff Scientist for ExxonMobil Technology Company, a sub-sidiary of Mobil Oil, where he was associated with research in the area of catalysis. He had worked for ExxonMobil for the past 21 years at Mobil's Paulsboro Technical Center in Paulsboro, New Jersey. A 1963 graduate of Anna-Jonesboro Community High School, John received his B.S. and M.S. in chemistry at Southern Illinois University in 1968 and 1970. He was an Officer in the 375th Aeromedical Evacuation Wing of the United States Air Force from 1970 to 1972 where he helped plan and coordinate hospital flights used for the evacuation of injured medical personnel from southeast Asia. He was accepted into the graduate studies program at Virginia Polytechnical Institute in 1972 and received his Ph.D. in Mineralogy and Geophysics from VPI in 1977. From 1977 to 1979 he pursued post-graduate work at the University of Chicago, Department of Geophysical Sciences. At the University of Chicago, John developed an interest in natural zeolites, a form of crystalline aluminosilicates that are used in detergents and as catalysts. He joined ExxonMobil at its Paulsboro Research Laboratory in 1979 as a crystallographer working in the areas of zeolites and progressed through various technical levels to the position of Senior Staff Scientist. John was the author or co-author of 40 journal publications and was an inventor on seven U.S. Patents. He was a member of the American Crystallographic Association.

Tom Degnan

Cathedrals and Synchrotrons for the 21st Century

Dedicated to the people of Dresden, Germany

We were walking in the *Place d'Armes* of *vieux* Montreal outside the *Notre Dame* Basilica after a brief visit inside. Although not very grandiose, this cathedral has harmonious architecture, and the light penetrating through beautiful glass-stained windows illuminated its interior and conveyed a peaceful and serene ambiance. The first and original chapel was a simple bark-covered structure built within the original city-fort in 1642. However, what we were looking at was of one the first cathedrals in Canada resulting from the Gothic Revival style designed by the Irish-American architect James O'Donnell and inaugurated in 1829(1). The occasion was the annual meeting of the ACA that took place in this Canadian City in August of 1995. There were three of us in the group: Cynthia Stauffacher, John Badger and yours truly. After our visit John uttered with some hidden regret in his voice:

-"We don't build these things any more",- referring to the unique cathedral in front of us.

Although I did not verbally respond right away, the thought occurred to me immediately:

-"No, we build synchrotrons instead."

The conversation went on to other things. Later in the day, I outlined in my mind the logic by which, as a scientist, I thought human kind in general and individual societies in particular are better off devoting their resources to constructing and developing large experimental facilities such as synchrotrons. In a sentence, the argument typically goes as follows: the scientific findings and technological developments obtained exploiting those large experimental facilities would revert back into society, resulting in a better standard of living. J. D. Bernal, the influential crystallographer and scientist who pioneered the early study of protein crystals by X-ray diffraction, was a great believer in the role that science should play in the improvement of the human condition (2). The societal commitment that is necessary to design and build dedicated storage rings-synchrotrons- for the production and use of X-rays for scientific investigation is enormous. The impact that they will have in our knowledge of the physical world in the next century and beyond is difficult to predict. As scientists, we do not question its critical role for the future of science, the public expense being analogous to an astronomical observatory, a particle accelerator or the space shuttle.

Those technological wonders are human artifacts that have practical value within the context of the secular and agnostic societies of today. Dedicated physicists, engineers, and instrument makers in accord with the scientific and technological goals of our societies build them; they are large projects funded by governments using tax revenues through their different agencies.

One might argue that cathedrals, on the other hand, were built in the Middle Ages by towns or 'burgs', strongly influenced by the religious beliefs and values dominant at the time. They constructed cathedrals as a way of '*rapprochement*', with the Lord almighty that provided the compass of their lives. They were erected in the middle of town by masons, artisans, carpenters and blacksmiths as a community effort, under the auspices of a bishop or religious leader. In our materialistic world of today we do not build those things any more. Or, do we?

One ordinary day, I received an invitation from Prof. H. Bernhart to the 5th European Congress of Medical Mycology to present a lecture on the structure of a protein secreted by the pathogenic fungus *Candida albicans*. This organism can cause very severe infections in people with a weakened immune system, such as people undergoing chemotherapy or patients diagnosed as HIV positive. The congress was going to take place in the city of Dresden, Germany in early spring. What caught my attention was that in the cover of the flier was an aerial view of what appeared to be a massive scaffold around a part of town that was basically in ruins. Who on earth would like to advertise a conference in a city that is undergoing massive reconstruction? What public relations firm had advised the organizers of the meeting to choose such a photo for the logo of the Conference? I asked for the necessary permissions and responded that I would be delighted to participate. I filed the brochure and the ensuing correspondence in a manila folder and went on to other things.

The confirmation letters arrived a few months later. I submitted a title for my contribution and a second circular arrived with more details about the congress. This time a different view of the same scaffold around the walls of a building being restored was displayed on the cover of the brochure for the congress. Winter gave way to spring and in preparation for the meeting I went to the *Encyclopaedia Britannica* to read some more background on Dresden, the capital of Saxony in Germany. It was well recognized that for centuries the city had been a center for music and musicians on a European scale. Important episodes of the life of Bach, Handel, and Teleman had taken place in Dresden. The city had often resonated in the past with the operas by Carl Maria von Weber, Richard Wagner and Richard Strausss. In addition to the unique examples of German baroque and rococo architecture, the picture galleries in the city included many works by old masters such as Holbein, Cranach, Vermeer, Rembrandt, Hals, van Dyck, Rubens, Botticelli and Canaletto. All of these were the 'treasures of Dresden' (3). Unfortunately, I also read the tragic details of the February 13-14, 1945 bombing that reduced the 'Florence on the Elbe' to rubble and ruins (3). The American writer Kurt Vonnegut Jr. survived the fire-bombing of the city as a prisoner of war with another infantryman Henry J. Leclair in an underground meat-locker, within the city slaughterhouse fifty feet underground. His chronicle of this infamous episode of World War II is iconoclastic, irreverent and cynical but at the same time is full of a profound human empathy (4). Within this historical framework, I began to understand the brochures of the conference a little bit better.

However, it was only when I set my footsteps in the city; when I walked down its streets and avenues and strolled down

continued on next page

the '*Altstadt*'; when I listened to music in the fully restored Semper Opera; when I indeed saw the rising walls of the '*Frauenkirche*', surrounded by a scaffold, and compared the view with old photographs of the city. Only then, I fully comprehended the significance of those proud walls growing inch by inch towards the full *wiederaufbau* of the city symbol from the devastation of World War II. Then, I fully understood why the photographs of the restoration were being proudly displayed in the posters announcing the Congress.

A few months after I wrote these ruminations regarding the restoration of the 'Florence on the Elbe' by their proud citizens -by then almost the end of twentieth century-, a ray of hope appeared in the horizon. Prof. Günter Blöbel (Rockefeller University, NY) winner of the 1999 Nobel Prize in Medicine and Physiology announced that he would donate the entire monetary award for the restoration of the *Frauenkirche* and a synagogue in Dresden (5). According to the report, Dr. Blöbel watched the devastation of the city as a child of eight from a few miles away and is the founder of a U.S. organization named 'Friends of Dresden' devoted to the restoration of the artistic treasures of that German city.

Upon further reflection, it also came to my mind the efforts to complete the cathedral or 'Templo de la Sagrada Familia' ('Temple of the Sacred Family') in Barcelona, Spain, the magnificent design of the Catalan architect Antoni Gaudí i Cornet (1852-1926). This cathedral more than any other that I know, represents an example of a basilica conceived, designed and being constructed in our time. Gaudí was not the original architect when the first stone was laid in 1882, however he accepted the commission in 1883 and would devote his entire life to it. The original architectural design of the temple is unique in many ways but this is not the place to expound on the details of the plans. I would like to invite the reader to visit it. Nonetheless, I want to focus on three aspects of this masterpiece (6).

First, the abundance of organic and biological forms in the design (7). Antoni Gaudí was the foremost representative of a school of architectural design (*Art Nouveau* in France or *Modernismo* in Catalonia) that reacted against the generic, geometric and linear forms of architecture at the beginnings of the 20th century. As to the overall design of the Sagrada Familia, Gaudí said that the nave, aisles and the vaults of the basilica should be 'like a forest' with light entering and flooding the windows. A forest accentuated by the twelve resonating bell towers reaching over 300 feet from the floor, four on each of the main facades and representing the apostles. Natural forms are displayed throughout: they are part of the crypt, the gargoyles and spires of the apse; plants and animals in the Nativity facade and fruits in the windows representing the different seasons of the year. A well-known detail is the presence of a turtle at the base of a column within the Portal of the Nativity façade; the poor creature

On the Cover:

Collage of Cathedrals and Synchrotrons

The current status of the Temple of 'La Sagrada Familia' (Barcelona, Spain) (upper left) and the 'vision' for the reconstruction of the Frauenkirche in Dresden, Germany (lower right). These images combined with aerial views of the Advanced Photon Source (APS, lower right, Argonne, Chicago, Illinois, U.S.A) and the European Synchrotron Radiation Facility (ESRF, Grenoble, France). I am grateful to Prof. Dr. Hannelore Bernhardt for her invitation to the 5th ECMM and for her hospitality during my visit to Dresden. I am also grateful for the enlarged view of the cover of the program for the Congress. The image is entitled 'Wiederaufbau der Frauenkirche in Dresden: Fotomontage des Kuntslers und Fotographen Jorg Schonet'. I must also thank my friends Dr. Jaume Olivella and Dr. María Angels García-Bach from Barcelona for the information and images about The Sagrada Familia. The assistance of Jim Sukowski and Jeff Frye of Abbott's Creative Network is appreciated for the preparation of the illustration. Images of APS and ESRF courtesy of their respective users office.

seems to support the entire structure. Second, color is ever present in Gaudí's architecture and the Sagrada Familia is no exception: the stained glass windows inside the temple and especially the mosaics and tiles as the terminations of the bell towers are fingerprints of the work of Gaudí. Finally the parish schools inside the cathedral that were built in 1909. As the architect expressed it: 'by the side of the Church, the people will receive education and culture'. This last detail makes the cathedral truly a community building. Although the schools were destroyed and part of the church sacked during the Spanish Civil War (1936-1939), the continuation and eventual completion of this masterpiece by the 21st century are on track. The financing is drawn from private contributions from all over the world and the work is about half completed. I can only wish that when the completed work is dedicated in the next century the name is changed from 'Temple of the Sacred Family' to 'Temple of the Human Family' (Templo de la Familia Humana). This minor change will put this magnificent cathedral in its rightful place as an icon of '*rapprochement*' of all human beings irrespective of their individual faiths and credos.

I should close these lines mentioning a scientific event related to synchrotrons that will have social, political and possibly historical implications. When time came to decommission the seventeen-year-old German synchrotron BESSY I (*Berliner Electronen-Speicherring fur Synchrotronstralung*), Herman Winick from the Stanford Linear Accelerator Center suggested the possibility of donating it to the Middle East region to foster scientific collaboration, and possibly as a seed for enduring peace. The idea has taken hold and UNESCO has given it a strong support. The plan would be to build an upgraded version and make it a centerpiece of collaborative research in various fields, among scientists from traditionally unfriendly nations (8). The eleven country members of SESAME (Synchrotron-light for Experimental Science and Applications in the Middle East) agreed on Christmas Eve 1999 to contribute the necessary funds to get the project started (9), and Jordan had been tentatively selected as a first-choice site for the facility (10). A location in Yerevan, Armenia (former Soviet Union) was chosen as a second choice. Besides technological artifacts, synchrotrons might prove to be instruments for peace in years to come(11). It is not the first time that rings have been used as symbols of peace and cooperation: remember the Olympic games.

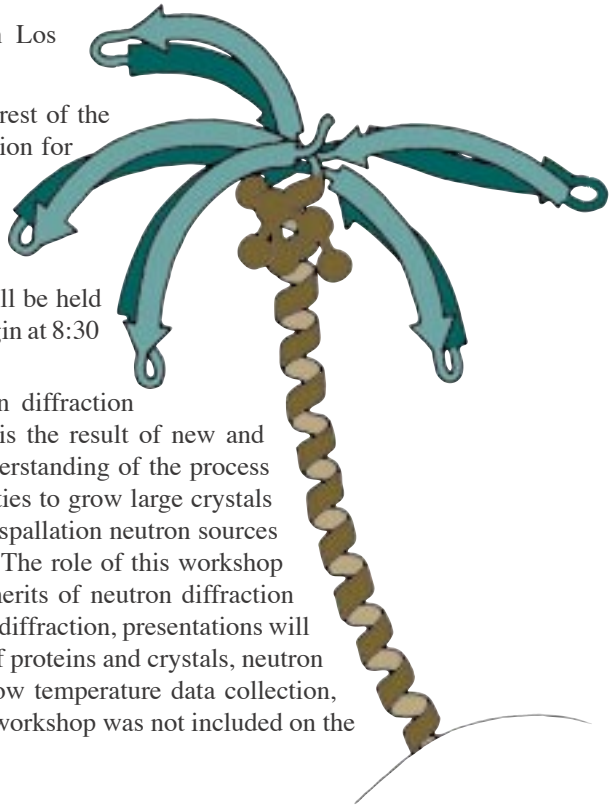
After putting all these recollections together, I realized that our casual, off-side and almost snobbish remark of a few years ago was only the reflection of one facet of the human persona. Our brain and our curiosity, combined with our internal logic, need to devise and construct probes to study the material world, in a constant struggle to understand its internal machinery and improve the human condition. Inextricably linked with this part of our minds -what we call our hearts and spirit- need to imagine, dream, write, play, paint, sculpt, chisel, mold and bend to overcome our fragility; to transcend our ephemeral nature, to make sense of our temporary passage through this earth. Then, let it be both: synchrotrons and cathedrals for a friendlier, more generous, increasingly fraternal and peaceful 21st Century, for all the inhabitants across planet Earth.

Notes

1. I would like to thank my friend in Montreal Ms. Laura Labrosse for helping me track down the exact place of my recollections and for sending me the information about the Notre Dame Basilica.

2. Bernal, J.D. (1969). *Science in History*. Three volumes. Pelican Books.
3. *Dresden 1945: The Devil's Tinderbox*. (Alexander McKee). E. P. Dutton, Inc. New York. 1984.
4. *Slaughterhouse-Five or The Children's Crusade*. 1969. Kurt Vonnegut. 25th anniversary edition. Delacorte Press/ Seymour Lawrence. 1994.
5. *Chemical & Eng. News*, October 18, 1999. Pg. 13-14.
6. The information is from brochures and publications about the 'Temple of the Sacred Family' sent to me by my dear friends Dr. Jaume Olivella and Dr. Maria Angels García-Bach from Barcelona.
7. Kemp, M. Science in culture. Inverted logic. Antonio Gaudí's structural skeletons for Catalan Churches. *Nature* (2000) 407: 838
8. T. Feder. German Synchrotron Light Source May Find New Home Somewhere in Middle East. *Physics Today*. August, 1999. Pg. 54.
9. T. Feder. Middle East Synchrotron Project Moves Ahead. *Physics Today.* February 2000. Pg. 52.
10. T. Feder. Jordan will likely Host Middle East Synchrotron Light Source. *Physics Today*. June 2000. Pg. 51.
11. SESAME Web site: http://www.sesame.org.jo

ACA '01 - July 21-26, 2001
Los Angeles, California



Preparations are well underway for the ACA's annual meeting in Los Angeles.

A fourth workshop has been added to the program (see below) and the rest of the program promises to be exciting and stimulating. Bring your suntan lotion for an wonderful week in California.

Neutron Diffraction Workshop

A fourth workshop entitled "Neutron Diffraction Studies of Macromolecules", organized by Gerry Bunick, Leif Hanson, and John Helliwell will be held Saturday, July 21, at the Westin Bonaventure Hotel. The workshop will begin at 8:30 a.m. The cost is $60 for registered students and $70 for all others.

The prospect is at hand for an exciting new era in biological neutron diffraction studies at steady state and spallation neutron sources worldwide. This is the result of new and upgraded neutron sources, advances in neutron detectors, and better understanding of the process of crystal growth. This confluence of events will provide both opportunities to grow large crystals on the International Space Station, and to collect data at steady state and spallation neutron sources such as ILL, JAERI, ISIS, LANSCE PCS, SNS, and the proposed ESS. The role of this workshop is to acquaint a new generation of protein crystallographers with the merits of neutron diffraction studies of macromolecules. Beyond providing a scientific case for neutron diffraction, presentations will include tutorials on large crystal growth, deuteration and perdeuteration of proteins and crystals, neutron data collection and refinement strategies, cooling of large crystals for low temperature data collection, and potential funding sources for neutron crystallography projects. This workshop was not included on the original registration form. An updated form is available on the website.

Program Chair: Duncan McRee (duncan.mcree@syrrx.com)
Local Chairs: Dan Anderson (dha@mbi.ucla.edu)
Katherine Kantardjieff (kkantardjieff@ exchange.fullterton.edu)

Getty Center Excursion

A Post-ACA meeting excursion to the Getty Center, one of the world's great masterworks of architecture (Richard Meier; gardens by Robert Irwin), has been planned. After the conclusion of the meeting, buses with luggage compartments will leave the Bonaventure Hotel at 1 pm July 26. The hilltop site provides panoramic views of the city, the Santa Monica Mountains, and the Pacific Ocean. The structures frame the views, the volumes, and the light. You could spend days on a pixel-by-pixel examination of the Getty Center, then days in the collections and exhibits. You will need comfortable shoes and sunglasses; it is literally and figuratively dazzling. Getty Center food services range from portable coffee carts to a restaurant (with an Alexis Smith installation) that requires reservations. Buses will leave the Getty Center parking garage at 5:30 pm, and take you and your luggage to Los Angeles International Airport or the buses can return you to the Bonaventure Hotel.

Registration Deadline..... June 1 Hotel Reservations Deadline..... June 18
Up To Date Information ..... www.hwi.buffalo.edu/ACA ACAAnnual/LosAngeles/

K.C. Cole to Receive the Elizabeth Wood Award

As stated in an earlier issue of the newsletter, K.C. Cole, a science writer for the Los Angeles Times, will receive the ACA's Elizabeth Wood Award at the 2001 meeting. This is in recognition of her writing about science for the public. She will give a presentation at the annual banquet in Los Angeles.

Cole spent her early childhood in Rio de Janeiro and grew up in Port Washington, New York and Shaker Heights, Ohio. After graduating from Barnard College with a BA in political science, she worked for Radio Free Europe as an editor, and subsequently lived in the former Czechoslovakia, Soviet Union and Hungary. She became a writer almost serendipitously when her piece on the aftermath of the Soviet invasion of Czechoslovakia appeared in the *New York Times Magazine*. While working as a writer and editor at the Saturday Review in San Francisco, she developed a love of physics through Frank Oppenheimer's Exploratorium and started writing about science – initially in the New York Times *Hers* column and a column in the Washington Post magazine. In the late 1970s, she became an editor at Newsday, and began writing personal essays on politics, humor and women's issues. Her first book, *What Only a Mother Can Tell You About Having a Baby*, was published by Doubleday in 1982. A collection of essays, *Between the Lines*, appeared two years later.

Since that time, Cole has been writing mostly about physics and mathematics for a wide variety of publications ranging from the *New York Times Magazine* and *Newsweek* to *Esquire* and *Lear's*. She wrote a column for *Discover* magazine when it was part of Time, Inc. in New York, and later became an editor for a subsequent incarnation of *Discover* under Disney in Los angeles. Since 1994, she has covered physical science for *The Los Angeles Times*, where she also writes the column, *Mind Over Matter*.

Cole's most recent book is an exploration of emptiness in all its philosophical, mathematical and physical richness. Published by Harcourt in January 2001, it is entitled *The Hole in the Universe: How Scientists Peered Over the Edge of Emptiness and Found Everything*.

She is also the author of the national best seller: *The Universe and the Teacup: The Mathematics of Truth and Beauty*, and also *First You Build a Cloud: Reflections on Physics as a Way of Life*. She has taught science writing as a Fellow at Yale and Wesleyan universities, and is currently Adjunct Professor of Science, Society and Communication at University of California at Los Angeles and Writer in Residence at the Institute for Practical and Applied Mathematics. She's an active member of JAWS (Journalism and Women Symposium) and a director of PEN West.

Among her recent awards are the American Institute of Physics Science Writing Award in 1995, the Skeptics Society Edward R. Murrow Award for Thoughtful Coverage of Scientific Controversies in 1998, and the Los Angeles Times award for deadline reporting, 1998, and the Los Angeles Times award for explanatory journalism, 1999.

We wish to thank the following Organizations for their support

BioCryst Pharmaceuticals, Inc.
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Hampton Research
International Union of Crystallography
Merck Research Laboratories
Molecular Structure Corp.
Nonius Company
Pharmacia Corp.
Procter & Gamble Pharmaceuticals, Inc.

TENTH ANNUAL ACA SUMMER COURSE IN CRYSTALLOGRAPHY

The tenth annual ACA Summer Course in Crystallography will be a 12 day course held from June 8 to June 20, 2001 at the University of Georgia, Athens GA.

The first seven days of the course will be devoted to basic crystallography of small molecules and will include lectures on the mathematics and physics behind structural analysis, the methods of structure solution, the refinement of atomic parameters and the presentation and analysis of the results of a structure determination. The laboratory associated with this part of the course will teach students to select and mount small molecule crystals, determine their unit cell dimensions and collect data on modern equipment. They will learn to use up-to-date crystallographic software packages to solve and refine structures. Finally, they will present a brief report on their results.

The final five days of the course will be devoted to macromolecular crystallography and include lectures on crystallization, data collection and processing, determination of heavy atom sites, structure solution by MIR, SIR, MAD, SAS and molecular replacement techniques, chain tracing, model building and refinement methods.

This year's Course will include Workshops on XtalVew with Duncan McRee, HKL2000 with Wladek Minor, and Single-wavelength Anomalous Scattering with Bi-Cheng Wang.

In addition, experienced laboratory instructors will be available for each of the laboratory sessions. The text chosen for the summer school is "Crystal Structure Analysis" by Glusker and Trueblood. A complete set of lecture notes will be provided to each student. Tuition for the 12 day Course is $800.00 if received before May 15th.

For more information please see the web site at:
http://bcl15.bmb.uga.edu/aca01/index.html or contact;
Dr. Gary Newton
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University of Georgia
Athens, GA 30602
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Fax: (706) 542 - 3077
E-mail: newton@chem.uga.edu

NOTE: APPLICATION FORMS MUST BE RETURNED TO DR. NEWTON BY May 6, 2001

Course Outline and Schedule

Day 0 Thursday, June 7 Lobby - Georgia Center
2:00 - 10:00 PM Arrival and Registration
DAY 1 Friday, June 8 Georgia Center
8:15 - 8:30 Welcome to Athens and Opening Remarks
8:30 - 9:30 Generation and Characteristics of X-rays
9:50 - 10:50 Preparation of Crystalline Samples
11:00 - 12:00 Unit Cells, Lattices and Miller Indices
1:30 - 5:00 Laboratory Sessions (locations to be announced)
7:00 - 9:00 Mathematics of Crystallography
DAY 2 Saturday, June 9 Georgia Center
8:30 - 9:30 Symmetry Elements
9:50 - 10:50 Space, Point and Laue Groups
11:00 - 12:00 Use of International Tables for Crystallography
1:30 - 5:00 Laboratory Sessions
6:00 - 9:00 Opening Mixer - food and drinks provided
DAY 3 Sunday, June 10 Georgia Center
8:30 - 9:30 X-ray Diffraction and the Reciprocal Lattice
9:50 - 10:50 Symmetry in the Reciprocal Lattice
11:00 - 12:00 Scattering by Single Atoms and Groups of Atoms
1:30 - 5:00 Laboratory Sessions
7:00 - 9:00 Q&A on previous three days of lectures
DAY 4 Monday, June 11 Georgia Center
8:30 - 9:30 Structure Factors, Fourier Transforms etc
9:50 - 10:50 Anomalous Scattering
11:00 - 12:00 Solving the Phase Problem
1:30 - 5:00 Laboratory Sessions
7:00 - 8:00 Instruments for Data Collection
DAY 5 Tuesday, June 12 Georgia Center
8:30 - 9:30 Patterson Methods
9:50 - 10:50 Data Collection Methods/Cryocrystallography
11:00 - 12:00 Processing Diffraction Data
1:30 - 5:00 Laboratory Sessions
7:00 - 8:00 Problem Structures
8:00 - 9:00 Crystal Twinning
DAY 6 Wednesday, June 13 Georgia Center
8:30 - 9:30 Direct Methods I
9:50 - 10:50 Direct Methods II
11:00 - 12:00 Structure Refinement by Least Squares
1:30 - 5:00 Laboratory Sessions
7:00 - 8:00 Historical Crystallography
DAY 7 Thursday, June 14 Georgia Center
8:30 - 9:30 Structural Info & Error Analysis
9:50 - 10:50 Structure Report and Publication
11:00 - 12:00 Structural Databases
1:30 - 5:00 ***** STUDENT PRESENTATIONS *****
7:00 - 9:00 BANQUET Georgia Center Banquet Area
After dinner "History of the ACA Summer School"
FRIDAY, JUNE 15 - Atlanta Sightseeing Trip!
MACROMOLECULAR SESSIONS
DAY 8 Saturday, June 16 Georgia Center
8:30 - 9:30 Crystallization of Macromolecules
9:50 - 10:50 Introduction to HKL2000

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11:00 - 12:00 Introduction to XtalView
1:30 - 5:00 Group A XtalView Workshop
1:30 - 5:00 Group B HKL2000 Workshop
1:30 - 5:00 Group C Crystallization/Data Collection Workshop
7:00 - 8:00 Crystallography on the International Space Station

DAY 9 Sunday, June 17 Georgia Center
8:30 - 9:30 Synchrotron Data Collection
9:50 - 10:50 Overview of MIR/SIR/MAD/SAD
11:00 - 12:00 Heavy Atom Derivatives & Location of HA Sites
1:30 - 5:00 Group B XtalView Workshop
1:30 - 5:00 Group C HKL2000 Workshop
1:30 - 5:00 Group A Crystallization/Data Collection Workshop
7:00 - 8:00 Maximum Likelihood
8:00 - 9:00 Crystallography of the Nucleic Acids

DAY 10 Monday, June 18 Georgia Center
8:30 - 9:30 MAD Theory
9:50 - 10:50 SAS Theory
11:00 - 12:00 Introduction to the ISAS Procedure
1:30 - 5:00 Group C XtalView Workshop
1:30 - 5:00 Group A HKL2000 Workshop
1:30 - 5:00 Group B Crystallization/Data Collection Workshop
7:00 - 8:00 Seminar - TBA

DAY 11 Tuesday, June 19 Georgia Center
8:30 - 9:30 Molecular Replacement
9:40 - 10:40 Model Building
11:00 - 12:00 Stereochemistry and Structural Parameters
1:30 - 3:30 Group A ISAS Workshop
3:40 - 5:40 Group B ISAS Workshop
7:00 - 8:00 High-Throughput Crystallography

DAY 12 Wednesday, June 20 Georgia Center
8:30 - 9:30 Refinement and Simulated Annealing
9:50 - 10:50 Structure Validation
11:00 - 12:00 The Protein Data Bank
1:30 - 3:30 Group C ISAS Workshop

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Determination of High-Resolution Structures for the Post-Genomic Age

June 3 - 17, 2001
Institute of Biochemistry and Biophysics, Warsaw, Poland
Institute of Bioorganic Chemistry, Poznan, Poland

With funding from the Howard Hughes Medical Institute, the U.S. National Research Council is sponsoring an intensive lab course for researchers from Central/Eastern Europe and the Newly Independent States. The first part of the course, devoted to macromolecular nuclear magnetic resonance (NMR), will be held at the Institute of Biochemistry and Biophysics in Warsaw, and the second part, concerned with macromolecular X-ray crystallography, at the Institute of Bioorganic Chemistry in Poznan. The aim of the course is to familiarize students with modern methods of macromolecular structure determination, including both X-ray crystallography and nuclear magnetic resonance (NMR) spectroscopy. The course will have theoretical as well as practical components involving actual crystallographic and NMR experiments, with opportunities for the participants' own projects. The course is designed for scientists from Central/Eastern Europe and the Newly Independent States who are in the early stage of their careers. Applicants should have the PhD or equivalent (kandidat), some background in molecular biology and/or biochemistry, and limited experience with structural methods. Highly qualified senior level graduate students who have not yet completed the PhD may apply provided they have the required background. English language proficiency is also required, as the course will be conducted only in English. Applicants must be citizens of one of the following countries: Albania, Armenia, Azerbaijan, Belarus, Bosnia-Hercegovina, Bulgaria, Croatia, Czech Republic, Estonia, Georgia, Hungary, Kazakhstan, Kyrgyzstan, Latvia, Lithuania, Macedonia, Moldova, Poland, Romania, Russia, Serbia-Montenegro, Slovakia, Slovenia, Tajikistan, Turkmenistan, Ukraine, and Uzbekistan. Students accepted to the course will receive tuition, course materials, and room and board free of charge. Free round-trip rail or air transportation between students' home cities and the course sites will also be provided.

For more detailed course information and application instructions, see http://www.nationalacademies.org/oia or contact Kelly Robbins - Fax: USA 202-334-2614; email: krobbins@nas.edu.

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Second International Workshop on Physical Characterization of Pharmaceutical Solids

September 23-28, 2001, Lancaster, PA, USA
Supported by Glaxo Wellcome, Cambridge Crystallographic Data Centre and Advanced Solid State Characterization, Inc.

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Dr. Michiel Van Oort, Glaxo Wellcome.
Dr. Marek Zakrzewski, Purdue Pharma.
Prof. Raj Suryanarayanan, University of Minnesota
Dr. Angeline Zakrzewski, ASSC Inc.

Purpose: Based on the success of the First International Workshop on Physical Characterization of Pharmaceutical Solids, the second workshop will be again designed to provide basic and in-depth understanding of modern physical characterization of pharmaceutical solids. The program is intended to benefit scientists and researchers in the areas of drug discovery, preformulation, formulation, stability testing, product development, product quality control, and analytical services. Workshop participants will be exposed to several analytical approaches for characterizing a solid. They will learn how these approaches can complement each other and be utilized individually or in concert in the solution of real problems in pharmaceutical development and solid state chemistry.

Objectives: The workshop will combine information about modern laboratory techniques to solve pharmaceutical problems and teach solid state characterization of pharmaceuticals. It will offer fundamental approaches as well as up-to-date technical information and future outlooks.

Who should attend?
The workshop is designed for scientists, formulators and regulatory personnel from pharmaceutical research and development companies, food processing firms, regulatory agencies, academia, analytical equipment manufacturers, and analytical laboratories.

Location: Eden Resort Inn, Lancaster, Pennsylvania, USA

Analytical Instrument Exhibition: A four-day commercial exhibition of analytical instrumentation is planned. Interested vendors are encouraged to reserve space. For more information please contact Advanced Solid State Characterization, Inc. under: Tel: (610) 594 2081 FAX (610)594 2082 E-mail: info@ASSCI.com

Abstracts: Abstracts for talks and posters must be received by ASSC Inc. no later than June 1, 2001. Authors should send contributions as computer files either by E-mail to info@ASSCI.com or mail on a 3.5 inch diskette together with an original and two copies of the hardcopy text, unfolded to ASSC, Inc. 520 Anthony's Drive, Exton, PA 19341 USA. Please use the template for abstract submission published at www.assci.com.

Presentations: Oral presentations will last 25 minutes including 5 minutes discussion. At the end of each session will be a 30 minute round table discussion.

Preliminary Topics: (including continuations of successful themes from IWPCPS-1 as well as new topics)
A Modern Pharmaceutical Solids State Laboratory
Polymorphism and How To Deal With It
Special XRD Applications
Modern Thermal Analysis Applications
Particle Size Analysis and Processing Effects on Product Performance
Morphology and Surface Characterization
Regulatory Patent Issues
Amorphous Content - Determination and Characterization
Solid State NMR Applications
Supercritical Fluids (Particle Design)
Expert Systems for Formulation Design (Informatics - Particle Engineering)
Drug Product Characterization
Characterization and Control of Dissolution
Bioavailability

Registration and Fees:
General registration until June 1, 2001: $1800
Late registration: $1950
Academic: $1200
A group discount is available, if more than three participatns from the same company register.
Electronic registration forms for the meeting and separate hotel accommodations are available at the meeting website (http://www.assci.com).

RUM 2000

Over 30 scientists from across the U.S. attended the 5th R-AXIS Users Meeting (RUM 2000) at the Woodlands Conference Center from November 10-12, 2000. In addition to the eleven invited lectures, several Molecular Structure Corporation employees gave talks on hardware, software and techniques in protein crystallography.

One of the recurring themes was that data collected in the home lab are still important for the solution of protein structures, even when synchrotron data are available. Speakers recounted experiences where data sets collected at home were at least as good as those obtained at a synchrotron, while others discussed experiments where the home lab data provided valuable or required assistance in solving structures with synchrotron data. Improved home lab equipment and techniques were also explored.

Recent developments in hardware and software arising from interest in high-throughput crystallography was another hot topic.

Lectures started on Saturday morning with opening remarks from MSC President Paul Swepston. Ron Stenkamp reported the heroic efforts required to obtain the 2.8 Å resolution structure of Rhodopsin, the first reported of a G-protein coupled receptor (GPCR). These GPCRs share many structural features, including a bundle of seven transmembrane alpha helices connected by six loops of varying lengths. The structure illustrated the interactions of the chromophore with a cluster of key residues that determine the wavelength of the maximum absorption. Changes in these interactions among rhodopsins facilitate color discrimination. Identification of a set of residues that mediate interactions between the transmembrane helices and the cytoplasmic surface, where G-protein activation occurs, also suggests a possible structural change upon photoactivation.

Kris Tesh discussed a number of new and old techniques for manipulating crystals and how to solve some of the problems often encountered with low temperature data collection. Steven Sheriff described tools such as beamstops, beam tunnels and cold stream alignment tools that had been designed or modified in their shop to speed up instrument alignment and data collection. He presented one dramatic case where a leak in the optics pathway led to such an increase in the background scatter that the cryo-pin was shadowed on the diffraction images.

Ann West presented a case where data carefully collected in her home lab produced the same results as synchrotron data, causing her to ask whether synchrotron trips are always necessary. Cheng Yang described his experiments using the anomalous signal from the sulfur atoms in heavy atom derivates to improve the phasing in a single wavelength protein structure analysis. Treating the sulfur anomalous data as a second heavy atom derivative, he was able to produce maps that were substantially easier to interpret than those from the heavy atom phases alone.

Fred Dyda reported two cases where experiments in his home lab were necessary to solve structures even though the primary data had been collected at a synchrotron. In one case an unexpected arsenic atom, originating from the cacodylate buffer during preparation of the Se-met derivative, contributed to the dispersive signal, making the maps uninterpretable until it was included.

Keith Crane introduced new hardware from his design group at MSC, including a new version of the X-stream low temperature system and an R-AXIS alignment stage, and Joe Ferrara presented information characterizing microsource

generators and new multilayer optics.

Bernie Santarsiero described different robotics systems developed by GNF, LBNL, Syrrx and Scripps and used in protein crystallization, automatic wet and dry sample mounting and crystal centering for high throughput crystallography. He showed videos of several systems in action. The crystallization robots utilized very small drop sizes with large numbers of simultaneous crystallization experiments.

Bog Stec started a very provocative discussion on the standardization of the methods of reporting structures. He called for better definitions of the diffraction limits of data deposited in the PDB.

A tour of the MSC facility was followed by dinner on Saturday evening.

The opening lecture on Sunday morning was by Zbyzek Otwinowski, who gave a detailed discussion of the errors in a diffraction experiment and how to get very high quality data by correcting for them during processing. He argued that home lab data is inherently better than synchrotron data because the demands on the goniometer and shutter are less stringent. He also demonstrated the value of Xenon derivatization for solving home lab data.

Craig Magee described his studies into the reaction centers in *Rhodopseudomonas spheroides*, showing how the use of different detergents and amphiphilic molecules as well as site-directed mutagenesis changed the intermolecular contacts and the crystallization properties of these membrane proteins. The comparison among the structure of wild-type and mutant proteins indicated the role of several residues and water molecules on the interface between proteins.

Phil Martin described the anisotropic refinement of ArsC at 1.6 Å using home lab data and Peter Nollert talked about the crystallization of intrinsic membrane positions in cubic lipid phases. The lipid can be made to stabilize the proteins in solution and guide their orientations. This technique has been used to grow crystals of the light-induced proton pump bacteriorhodopsin from the plasma membrane of *Halobacterium salinarum* that diffract to 1.9 Å. Practical tips on setting up such crystallization conditions and ideas to minimize the amount of protein required were presented.

S. Ramaswamy showed how to detect merohedral twinning in proteins using visual inspection with a microscope and intensity statistics. He demonstrated methods for determining the twin fraction using statistical methods and information from an untwinned data set.

Two software talks closed out the session and the meeting, with lectures given by John Edwards (CrystalClear) and Jim Pflugrath (automated data acquisition and processing for area detectors).

Bev Vincent

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Meeting Calendar

In order to conserve space and paper, contact points for most meetings announced in previous newsletter issues will not be repeated. More complete information can be found in back issues of the newsletter.

JUNE 2001

3-17 Determination of High-Resolution Structures for the Post-Genomic Age. Institute of Biochemistry and Biophysics, Warsaw, Poland, Institute of Bioorganic Chemistry, Poznan, Poland. For information and application instructions, see www.nationalacademies. org/oia or contact Kelly Robbins - Fax: USA 202-334-2614; email: krobbins@nas.edu.

8-20 2001ACA Summer Course in Crystallography, Athens, GA. Georgia Center for Continuing Education, University of Georgia. http://BCL15.bmb.uga.edu/aca2k.html

JULY 2001

21-26 ACA '01 Los Angeles, CA. Local Chairs: Katherine Kantardjieff (CSU-Fullerton, kkantardjieff@exchange.fullterton.edu) and Dan Anderson (UCLA, dha@mbi.ucla.edu). Program Chair: Duncan McRee (Syrrx, duncan.mcree@syrrx.com). Meeting website: www.hwi.buffalo.edu/ACA/ACA-Annual/LosAngeles/.

30-August 3 50th Annual Denver X-ray Conference. Sheraton Steamboat Resort, Steamboat Springs, Colorado, USA For information contact: Conference Coordinator International Centre for Diffraction Data 12 Campus Boulevard, Newtown Square, PA 19073 Tel: (610) 325-9814 Fax: (610) 325-9823 E-mail: dxc@icdd.com Web-site: www.dxcicdd.com.

SEPTEMBER 2001

23-28 International Workshop on Physical Characterization of Pharmaceutical Solids (IWPCPS-2). Lancaster, PA, USA. Contact: Chris Stoner Marketing Assistant ASSC, Inc. info@assci.com.

MAY 2002

25-30 ACA '02 San Antonio, TX. Local Chairs: Ray Davis (UT Austin) and Marv Hackert (UT Austin, m.hackert@ mail.utexas.edu). Program Chair: Wally Cordes (Arkansas, wcordes.comp.uark.edu).

AUGUST 2002

6-15 19th IUCr General Assembly and Intl. Congress of Crystallography. Jerusalem, Israel. Contact: J. Bernstein, Ben Gurion University, Beer Sheva, Israel.

Positions Available

It is expected that the employers listed in this publication are equal opportunity employers who wish to receive applications from qualified persons regardless of age, national origin, race, religion, sex or physical handicaps. Please inform the Editor when the positions are filled, and of any positions that do not give opportunities to all applicants. Ads will appear in two successive newsletters unless the Editor is notified that the advertisement should be continued longer or discontinued earlier.

For the most up-to-date listings check the ACA Home Page under the Positions Vacant heading. http://www.hwi.buffalo.edu/ACA/

Postdoctoral Position in Crystallographic Phasing Methods

Cornell High Energy Synchrotron Source (CHESS) is seeking a postdoctoral research associate in an interdisciplinary area of new phasing-method developments in x-ray protein crystallography. This position is being funded through a collaboration with Hauptman-Woodward Institute in Buffalo, NY. The main goal of the project is to develop new phasing capabilities with direct measurements of Bragg-reflection phases in x-ray crystallography experiments, and to apply the new algorithms to structural determination of proteins and other complex materials. A successful candidate should have a Ph.D. in a physical-science field, and experience in one or more of the following areas: synchrotron x-ray diffraction experiments, structural determination of proteins or complex small molecules, and programming in phasing methods and/or experimental data reduction and analysis. The position is intended for two years with a possibility of renewal for another 2-yr term. Interested applicants should send a curriculum vita, a list of publications, and names of at least three references to: Dr. Qun Shen, Cornell High Energy Synchrotron Source (CHESS), Wilson Laboratory, Cornell University, Ithaca, New York 14853, Phone: 607-255-0923, Fax: 607-255-9001, E-mail: qs11@cornell.edu., URL: http://www.chess.cornell.edu

Positions Previously Listed

Inorganic Chemist - Crystallographer

A post-doctoral position is available for a person skilled in both inorganic synthesis and X-ray crystal structure determinations. Send resume and a letter of recommendation to: Prof. Abraham Clearfield, Department of Chemistry, Texas A&M University, P.O. Box 30012, College Station, Texas 77842-3012, Clearfield@mail.chem.tamu.edu.

Biological Macromolecular Crystallographer

The Biomolecular Structure Teaching and Research program of the University of Saskatchewan is seeking an X-ray crystallographer to fill a tenure-track assistant professor position in the Dept. of Chemistry, with associate membership in the Dept. of Biochemistry. Further information can be found on the Internet at www.usask.ca/chemistry/ and www.usask.ca/medicine/biochemistry/.

Assistant or Associate Project Scientist

A position of Assistant or Associate Project Scientist is available for a Protein Crystallographer to work on the structure of the complex of the cAMP dependent Protein Kinase (PKA) with its Anchoring Protein (AKAP). Excellent working and living conditions. Salary ($50-70K) depending on background and experience. Please send resume and names of 3 references to: Prof. Nguyen-huu Xuong, Dept. of Chem. & Biochem., UCSD, 9500 Gilman Dr., La Jolla, CA 92093-0359; or to Prof. Susan Taylor, Dept. of Chem. & Biochem,. UCSD, 9500 Gilman Dr. La Jolla, CA 92093-0654.

Postdoctoral Research Associates

The Biology Department and National Synchrotron Light Source at Brookhaven National Laboratory seek two Postdoctoral Research Associates. The first of these will study the direct solving of macromolecular crystal structures through measurement of phases by multiple-beam diffraction methods (http://x12wulfgar01.nsls.bnl.gov/3BD/3beam_diffraction.html). The research associate will join an international collaboration on method development and application of multiple-beam phasing, and will be part of a large community of macromolecular crystallographers and diffraction physicists at BNL. A new six-circle diffractometer, equipped with a Quantum-4 area detector is available for the work; ample beam time will be available. This is an excellent opportunity for a candidate who has a Ph.D. in an appropriate field and established credentials in crystallographic studies. Additional experience in diffraction physics and macromolecular crystallography will be an advantage. More information about the position can be obtained from Robert Sweet (sweet@bnl.gov) or Dieter Schneider (schneider@bnl.gov). Applicants should send a curriculum vitae, a list of publications, and names of at least three references to Marsha Kipperman, Bldg. 185, BNL, Upton, NY 11973. Reference Position 9107.

The other Postdoctoral Research Associate will participate in technological developments at the National Synchrotron Light Source for rapid throughput macromolecular structure determination. The work will involve development of robotics for the handling of crystals under cryogenic conditions, work on a massively parallel computing cluster, and commissioning of new x-ray optical systems. The worker will be part of a large community of macromolecular crystallographers and diffraction physicists at BNL. This community includes an NIH-funded Protein-Structure Initiative consortium (http://www.nysgrc.org/) and an active and well funded program in facilities operation and development (http://www.x12c.nsls.bnl.gov/x12c/nsls_px.html). This is an especially nice opportunity for a candidate who has a Ph.D. in an appropriate field, established credentials in electromechanical design and implementation, and unix system programming. Additional experience in diffraction physics and macromolecular crystallography will be an advantage. More information about the position can be obtained from Dieter Schneider (schneider@bnl.gov) or Robert Sweet (sweet@bnl.gov). Applicants should send a curriculum vitae, a list of publications, and names of at least three references to Marsha Kipperman, Bldg. 185, BNL, Upton, NY 11973. Reference Position 9108.